Entropy and Experimental Design

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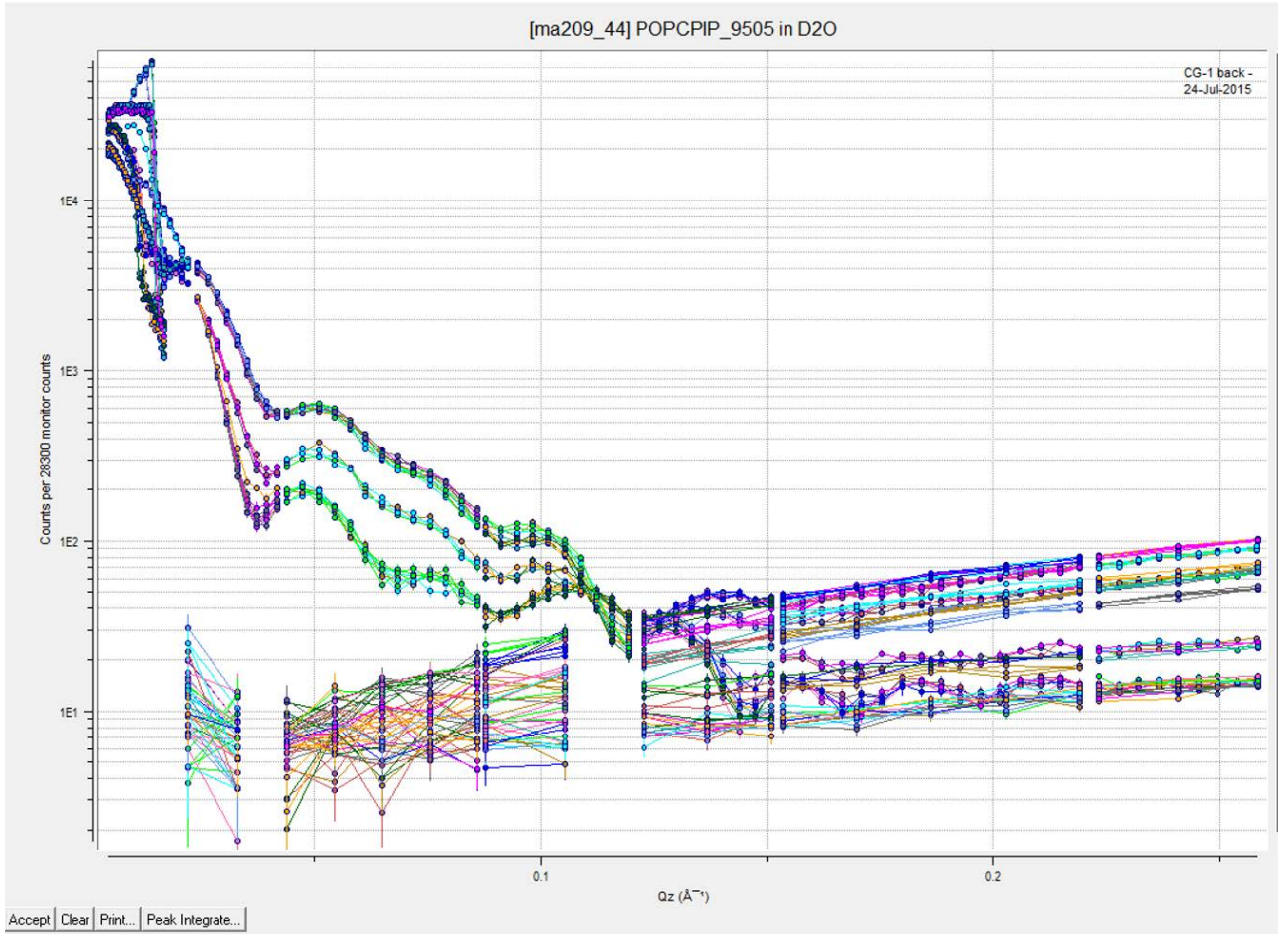
Motivation

- Measurement is expensive and time consuming
- We want to optimize the amount of information from an experiment against the cost of performing the experiment

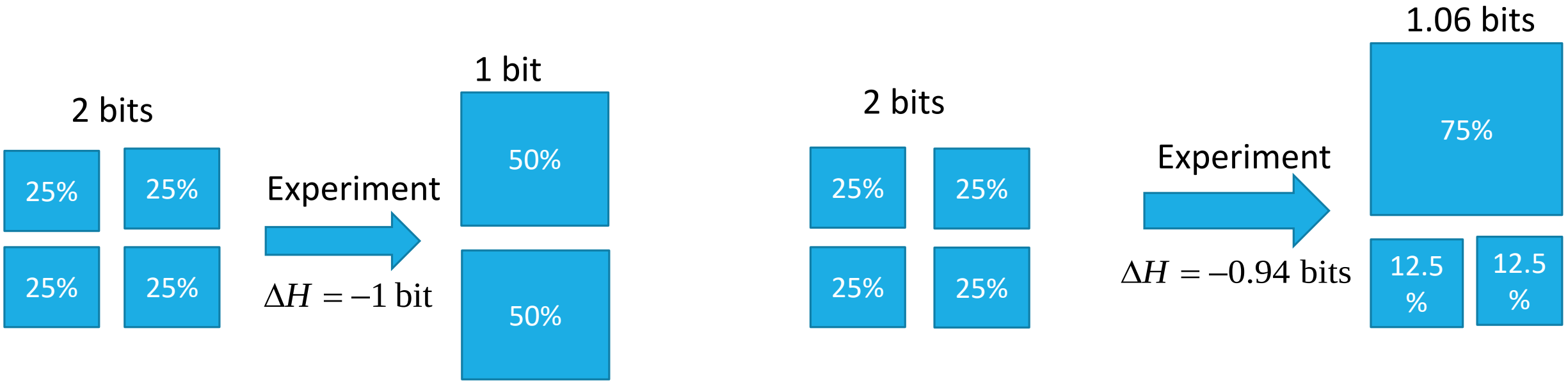


HIV GAG protein data from Magik

Information—Shannon Entropy

$$H(X) = -\sum_{i \in X} p(x_i) \log_2 p(x_i)$$

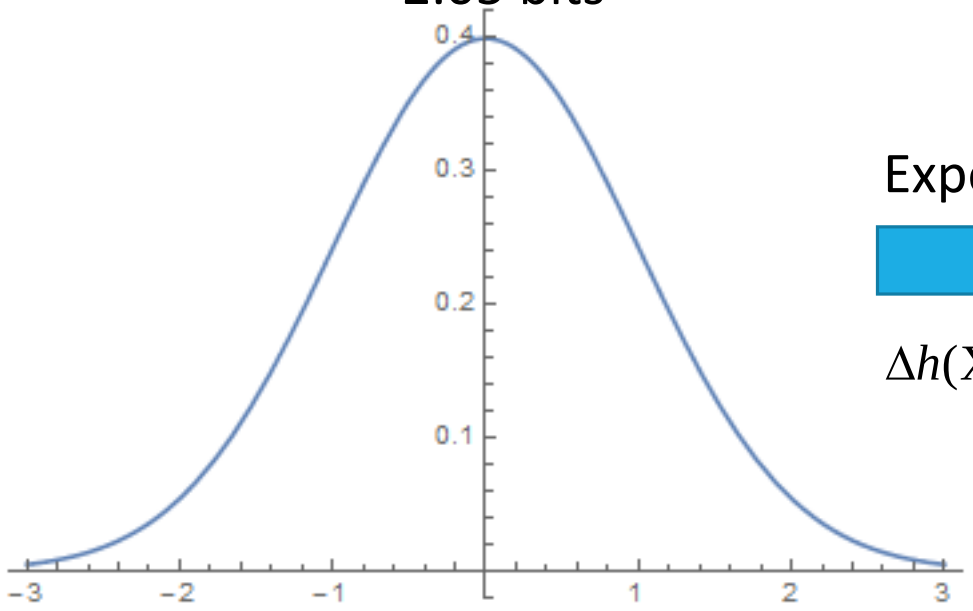
$H(X) = \log_2 n$ if p is a uniform distribution



Information—Differential Entropy

$$h(\mathrm{X})=\int_X p(x)\log_2 p(x)dx$$

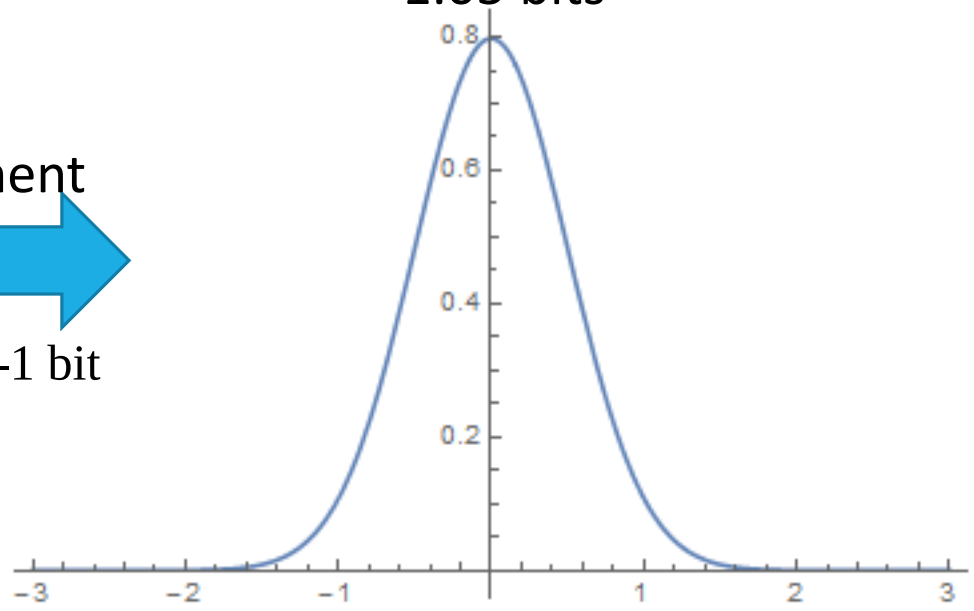
2.05 bits



Experiment

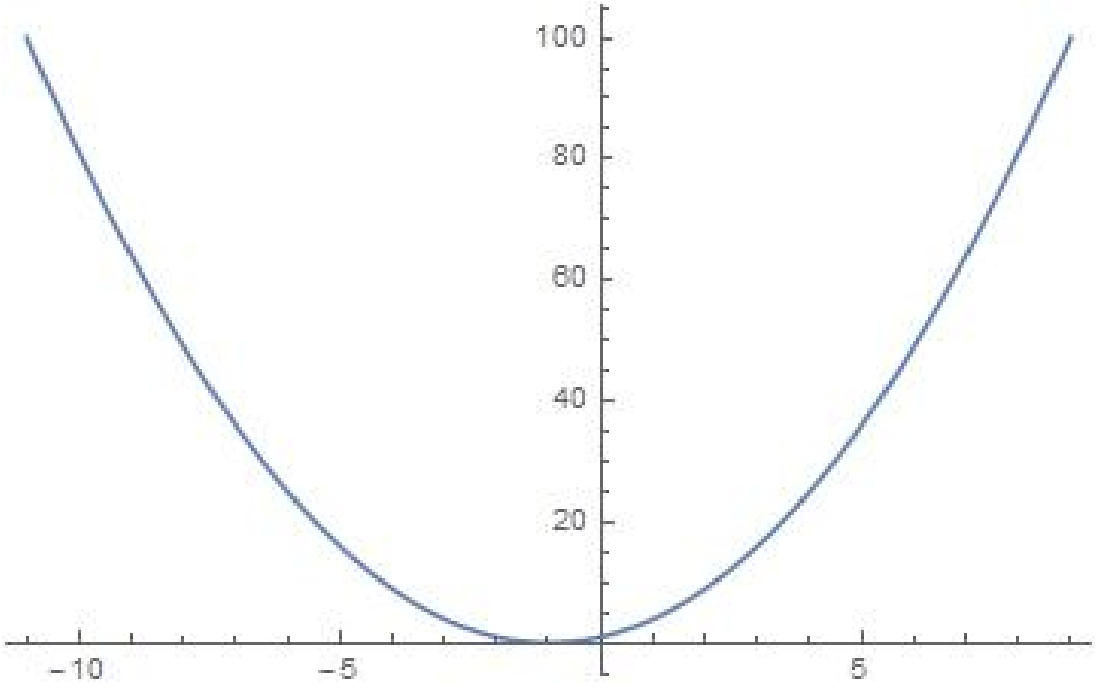
$\Delta h(\mathrm{X}) = \text{-1 bit}$

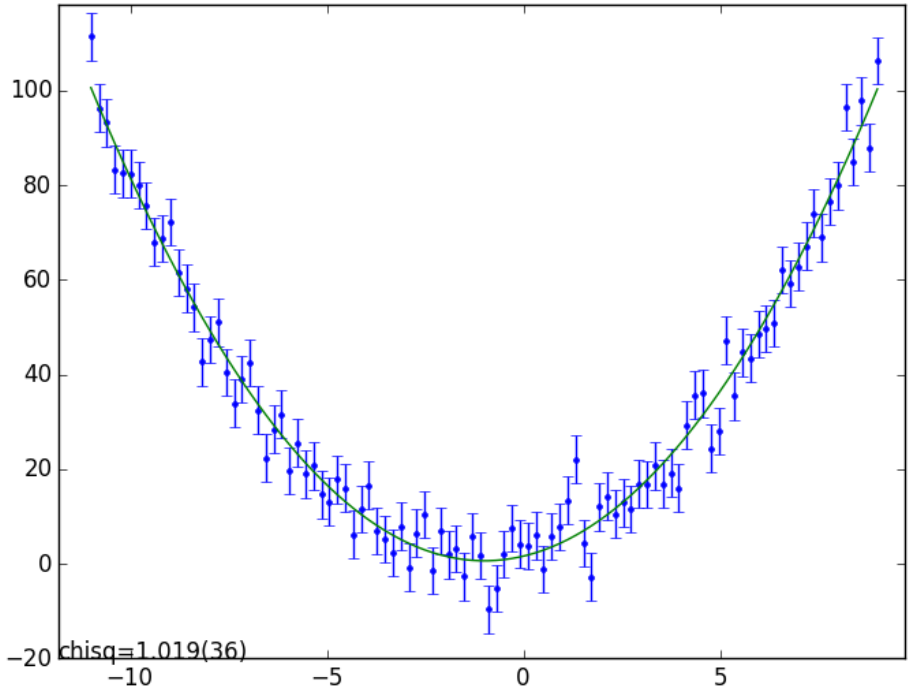
1.05 bits



Bumps Example

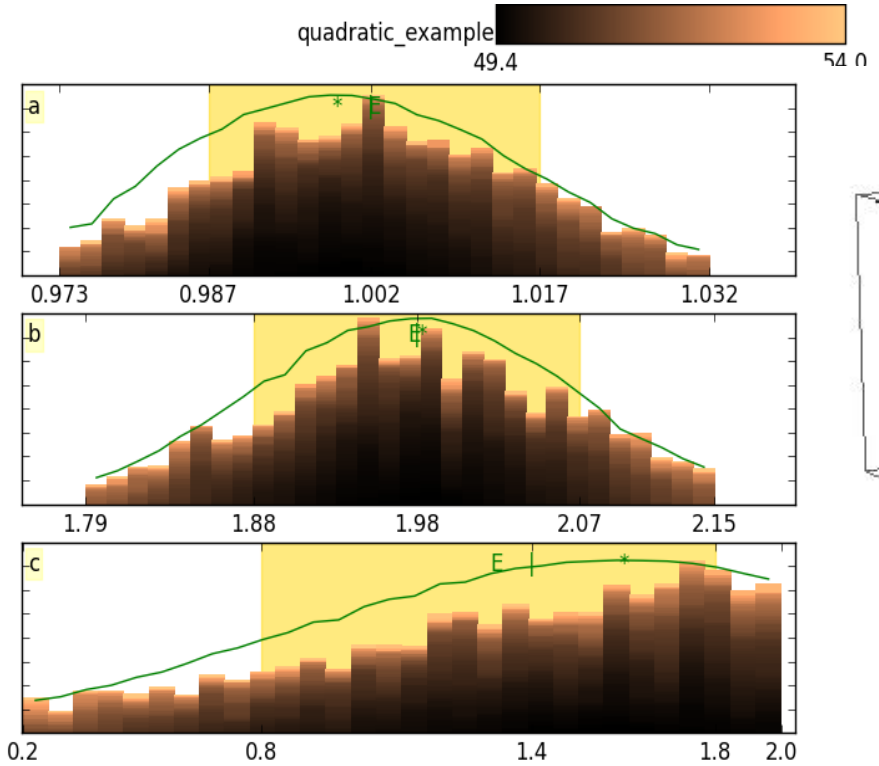
- Create a model for experiment and simulate data

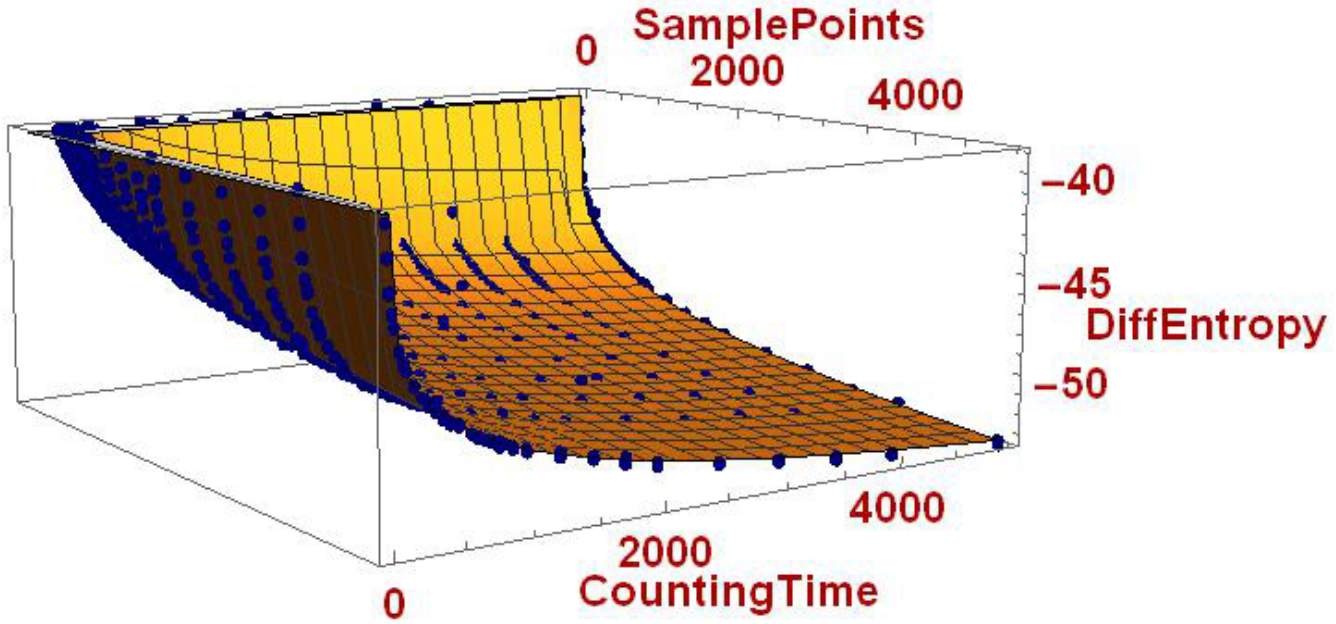




Bumps Example

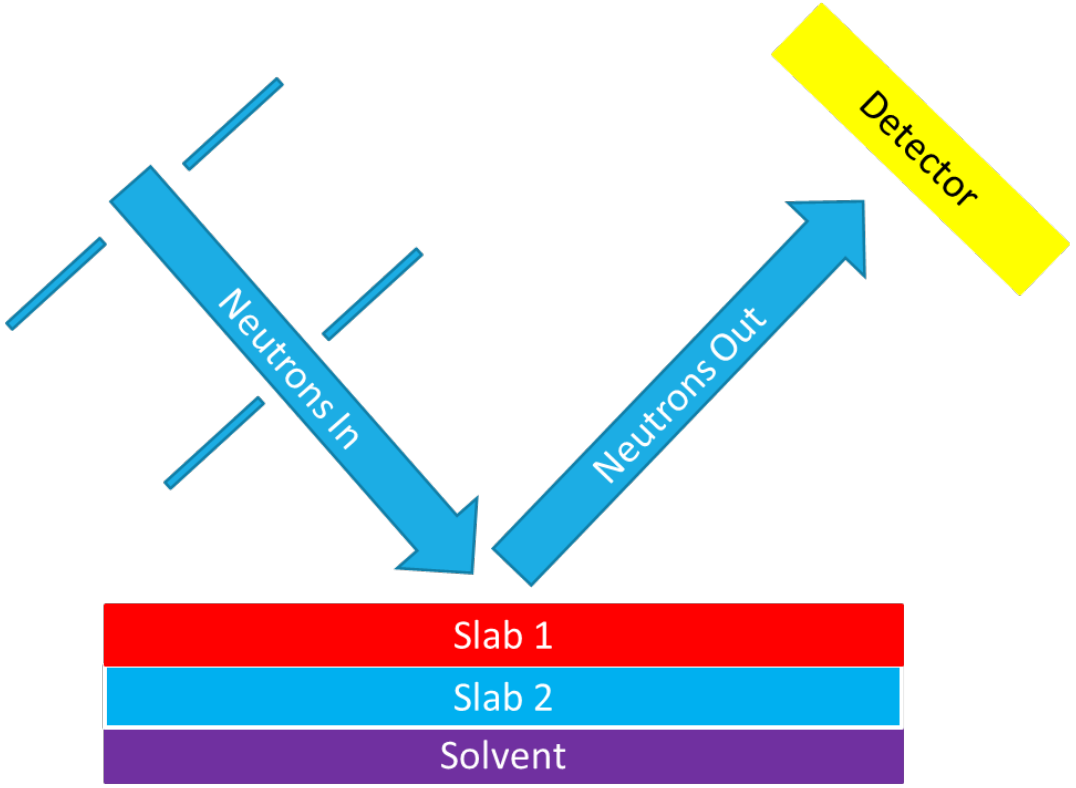
- Fit the data and calculate the entropy on the posterior distributions



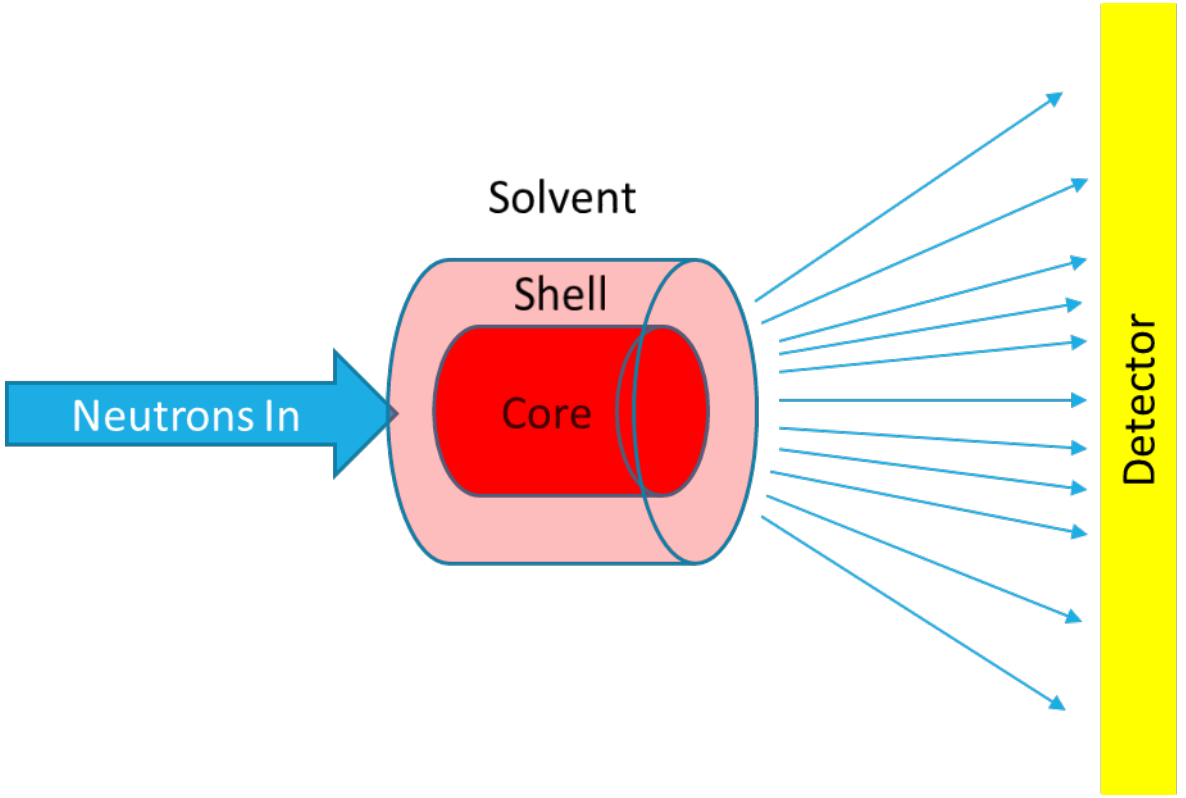


Reflectivity and SANS Model

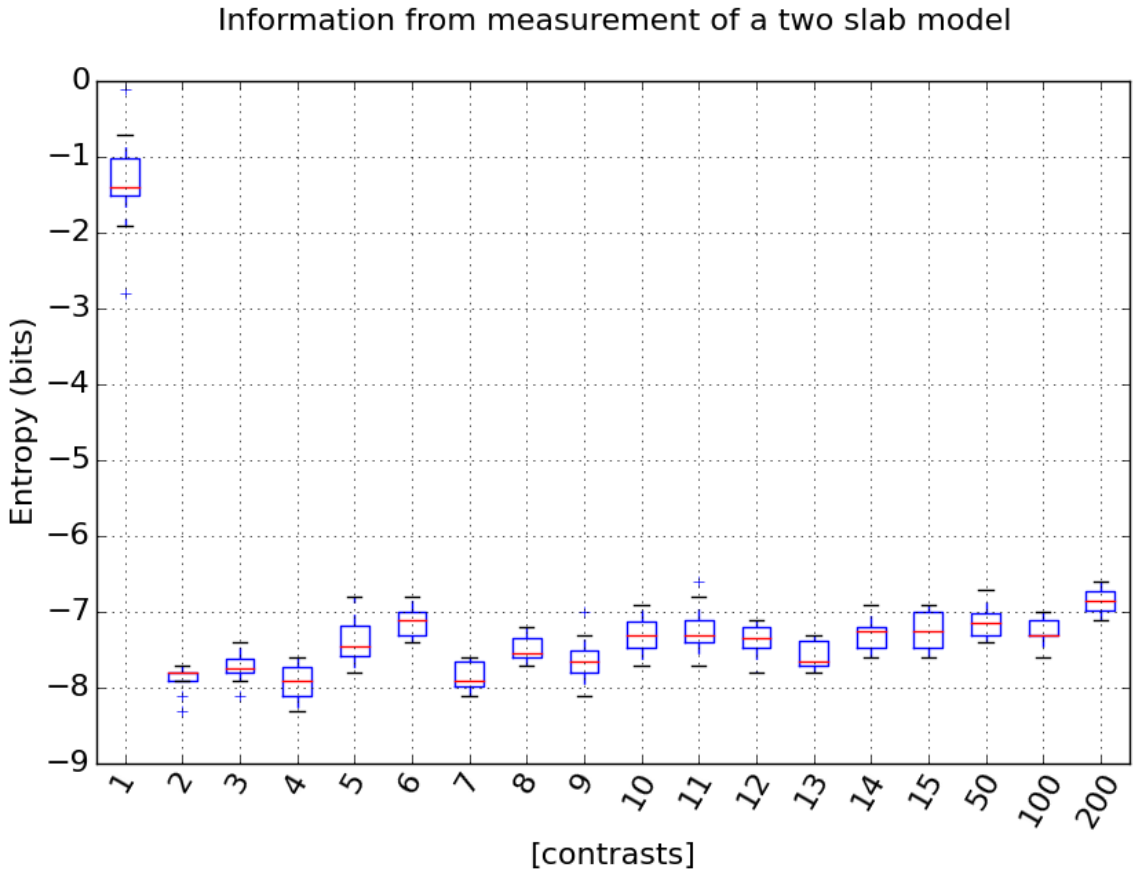
Reflectivity

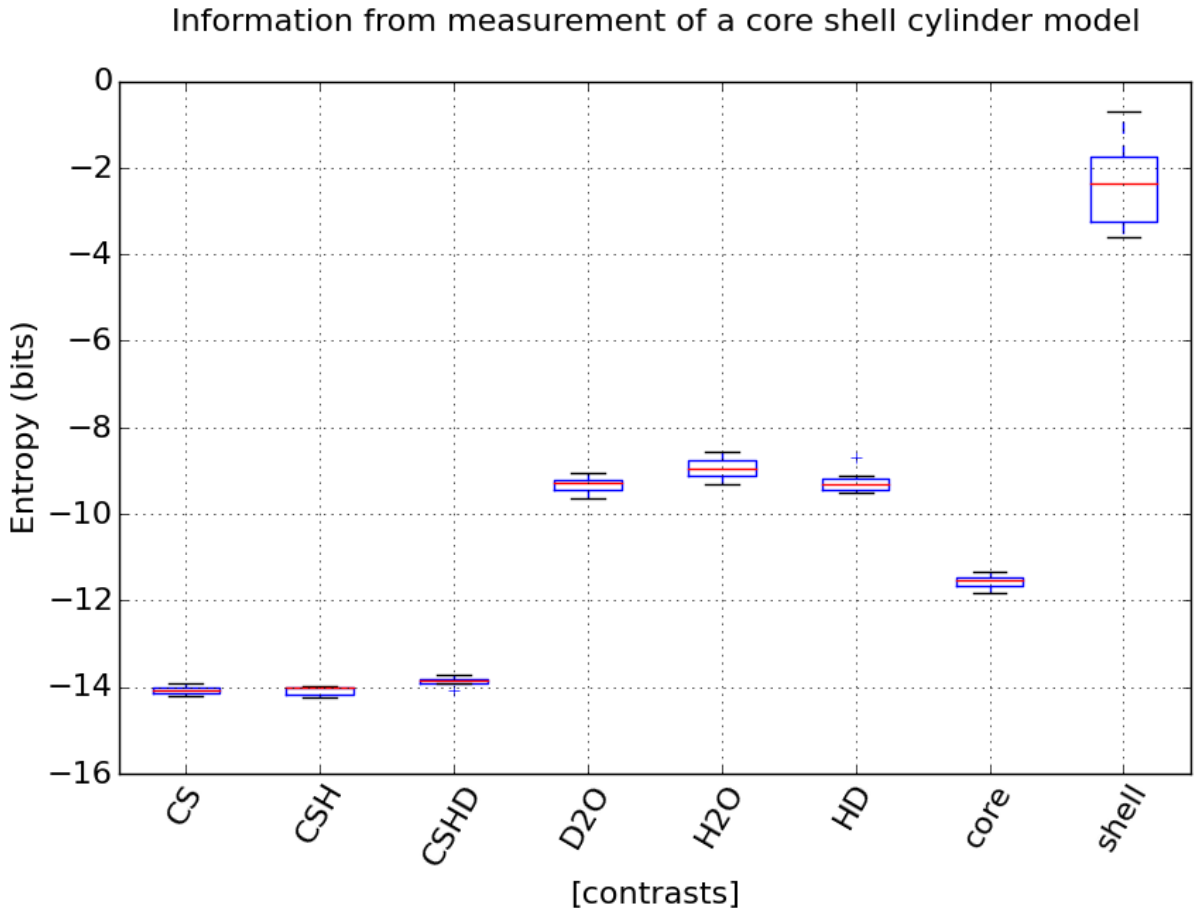


Small Angle Neutron Scattering (SANS)



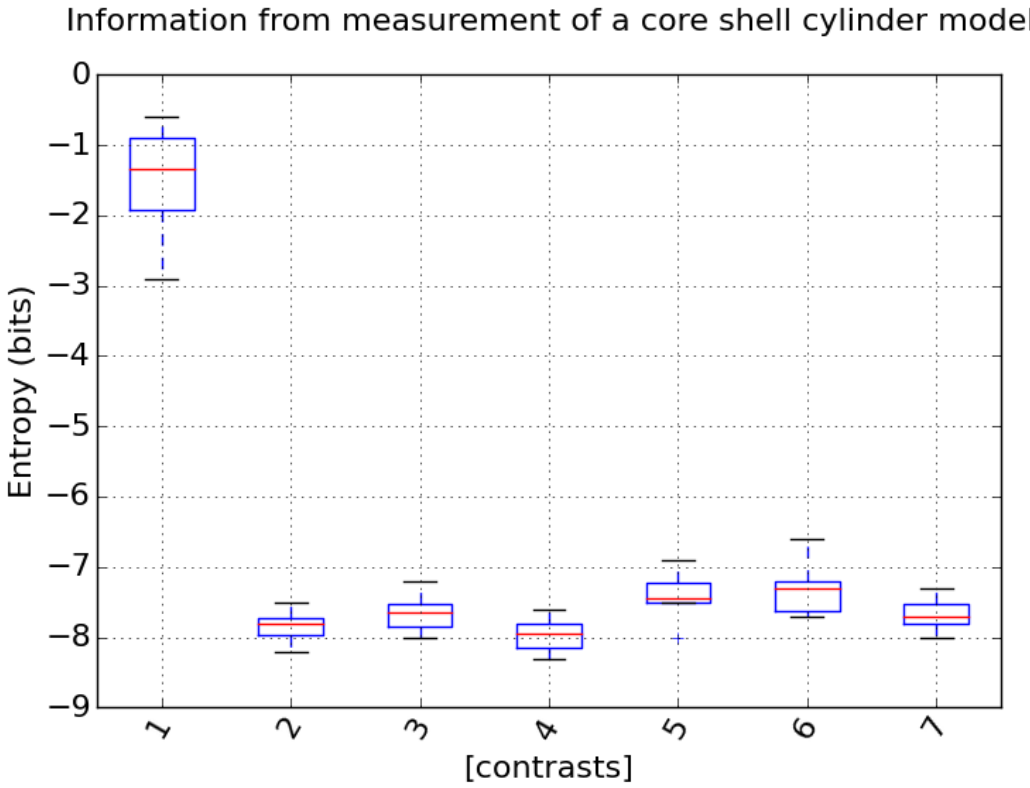
Reflectivity and SANS Entropy

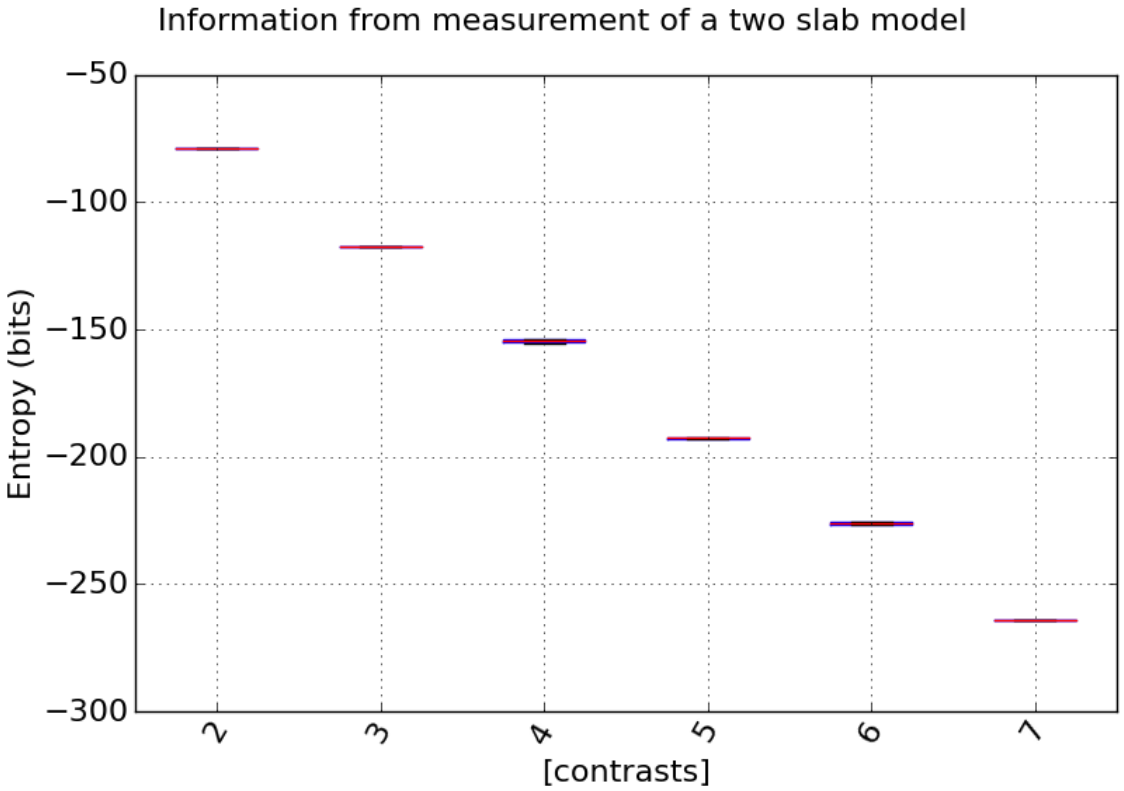




Reflectivity with Nuisance Parameters

- Entropy decreases linearly with number of contrasts





Future Work

- Improve entropy calculations for large numbers of parameters
- Investigate why the reflectivity model causes entropy to decrease linearly as the number of contrasts grows
- Investigate influence of number of parameters on entropy calculations
- Apply entropy to more interesting reflectivity problems and other experiment types

Acknowledgments

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